

## NAME

Fsp3CarbonsDescriptors

## SYNOPSIS

```
use MolecularDescriptors::Fsp3CarbonsDescriptors;

use MolecularDescriptors::Fsp3CarbonsDescriptors qw(:all);
```

## DESCRIPTION

Fsp3CarbonsDescriptors class provides the following methods:

new, GenerateDescriptors, GetDescriptorNames, StringifyFsp3CarbonsDescriptors

Fsp3CarbonsDescriptors is derived from MolecularDescriptors class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in Fsp3CarbonsDescriptors, MolecularDescriptors or ObjectProperty classes using Perl's AUTOLOAD functionality. These methods are generated on-the-fly for a specified object property:

```
Set<PropertyName>(<PropertyValue>);
$PropertyValue = Get<PropertyName>();
Delete<PropertyName>();
```

Fraction sp3 carbons (Fsp3Carbons) [ Ref 115-116, Ref 119 ] value is calculated by dividing the number of sp3 carbons (Sp3Carbons) with the total number of carbons in a molecule.

## METHODS

new

```
$NewFsp3CarbonsDescriptors = new MolecularDescriptors::
    Fsp3CarbonsDescriptors(%NamesAndValues);
```

Using specified *Fsp3CarbonsDescriptors* property names and values hash, new method creates a new object and returns a reference to newly created Fsp3CarbonsDescriptors object. By default, the following properties are initialized:

```
Molecule = ''
Type = 'Fsp3Carbons'
@DescriptorNames = ('Fsp3Carbons', 'Sp3Carbons')
@DescriptorValues = ('None', 'None')
```

Examples:

```
$Fsp3CarbonsDescriptors = new MolecularDescriptors::Fsp3CarbonsDescriptors(
    'Molecule' => $Molecule);

$Fsp3CarbonsDescriptors = new MolecularDescriptors::Fsp3CarbonsDescriptors();

$Fsp3CarbonsDescriptors->SetMolecule($Molecule);
$Fsp3CarbonsDescriptors->GenerateDescriptors();
print "Fsp3CarbonsDescriptors: $Fsp3CarbonsDescriptors\n";
```

GenerateDescriptors

```
$Fsp3CarbonsDescriptors->GenerateDescriptors();
```

Calculates Fsp3Carbons and Sp3Carbons values for a molecule and returns *Fsp3CarbonsDescriptors*.

GetDescriptorNames

```
@DescriptorNames = $Fsp3CarbonsDescriptors->GetDescriptorNames();
@DescriptorNames = MolecularDescriptors::Fsp3CarbonsDescriptors::
    GetDescriptorNames();
```

Returns all available descriptor names as an array.

StringifyFsp3CarbonsDescriptors

```
$String = $Fsp3CarbonsDescriptors->StringifyFsp3CarbonsDescriptors();
```

Returns a string containing information about *Fsp3CarbonsDescriptors* object.

## AUTHOR

Manish Sud <msud@san.rr.com>

## SEE ALSO

MolecularDescriptors.pm, MolecularDescriptorsGenerator.pm

## COPYRIGHT

Copyright (C) 2015 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.